

Dechant, Pierre-Philippe ORCID:

<https://orcid.org/0000-0002-4694-4010> (2014) Affine symmetry principles for non-crystallographic systems & applications to viruses/carbon onions. In: 30th International Colloquium on Group Theoretical Methods in Physics, 14th - 18th July 2014, Ghent University, Ghent, Belgium. (Unpublished)

Downloaded from: <http://ray.yorks.ac.uk/id/eprint/4016/>

Research at York St John (RaY) is an institutional repository. It supports the principles of open access by making the research outputs of the University available in digital form. Copyright of the items stored in RaY reside with the authors and/or other copyright owners. Users may access full text items free of charge, and may download a copy for private study or non-commercial research. For further reuse terms, see licence terms governing individual outputs. [Institutional Repository Policy Statement](#)

# RaY

Research at the University of York St John

For more information please contact RaY at [ray@yorks.ac.uk](mailto:ray@yorks.ac.uk)



Durham  
University



# Affine symmetry principles for non-crystallographic systems & applications to viruses/carbon onions

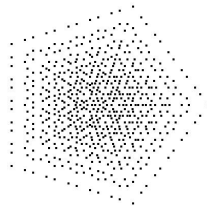
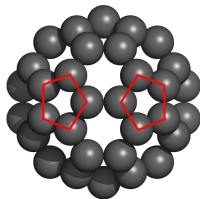
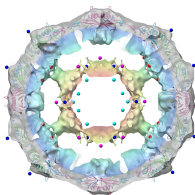
Pierre-Philippe Dechant

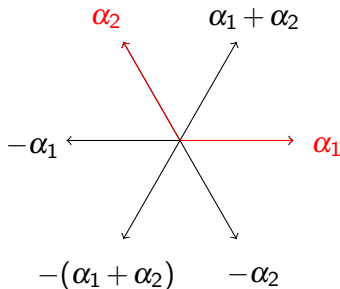
Mathematics Department, Durham University  
Work with [Reidun Twarock](#) (York) and [Céline Böhm](#) (Durham)

30th International Colloquium on Group Theoretical Methods  
in Physics, Ghent – July 17, 2014

# Motivation: Viruses

- Geometry of **polyhedra** described by **Coxeter** groups
- Viruses have to be '**economical**' with their **genes**
- Encode **structure** modulo **symmetry**
- **Largest discrete symmetry of space** is the **icosahedral** group
- Many other '**maximally symmetric**' objects in nature are also icosahedral: **Fullerenes & Quasicrystals**
- But: viruses are not just polyhedral – they have **radial structure**. **Affine extensions** give **translations**



Root systems –  $A_2$ 

**Root system**  $\Phi$ : set of vectors  $\alpha$  such that

$$\Phi \cap \mathbb{R}\alpha = \{-\alpha, \alpha\} \quad \forall \alpha \in \Phi$$

and  $s_\alpha \Phi = \Phi \quad \forall \alpha \in \Phi$

**Simple roots**: express every element of  $\Phi$  via a  $\mathbb{Z}$ -linear combination (with coefficients of the same sign).



# Cartan Matrices

Cartan matrix of  $\alpha_i$ s is 
$$A_{ij} = 2 \frac{(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = 2 \frac{|\alpha_j|}{|\alpha_i|} \cos \theta_{ij}$$

# Cartan Matrices

Cartan matrix of  $\alpha_i$ s is

$$A_{ij} = 2 \frac{(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = 2 \frac{|\alpha_j|}{|\alpha_i|} \cos \theta_{ij}$$

angles

$$\cos^2 \theta_{ij} = \frac{1}{4} A_{ij} A_{ji}$$

lengths

$$l_j^2 = \frac{A_{ij}}{A_{ji}} l_i^2$$

$$A_{ii} = 2$$

$$A_{ij} \in \mathbb{Z}^{\leq 0}$$

$$A_{ij} = 0 \Leftrightarrow A_{ji} = 0.$$

$$A_2: A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

# Cartan Matrices

Cartan matrix of  $\alpha_i$ s is  $A_{ij} = 2 \frac{(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = 2 \frac{|\alpha_j|}{|\alpha_i|} \cos \theta_{ij}$

angles  $\cos^2 \theta_{ij} = \frac{1}{4} A_{ij} A_{ji}$  lengths  $l_j^2 = \frac{A_{ij}}{A_{ji}} l_i^2$

$$A_{ii} = 2 \quad A_{ij} \in \mathbb{Z}^{\leq 0} \quad A_{ij} = 0 \Leftrightarrow A_{ji} = 0.$$

$$A_2: A = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

Coxeter-Dynkin diagrams: node = simple root, no link = roots orthogonal, simple link = roots at  $\frac{\pi}{3}$ , link with label  $m$  = angle  $\frac{\pi}{m}$ .

$$A_2 \circ \text{---} \circ \quad H_2 \circ \overset{5}{\text{---}} \circ \quad I_2(n) \circ \overset{n}{\text{---}} \circ$$

# Coxeter groups

A **Coxeter group** is a group generated by some **involutive generators**  $s_i, s_j \in S$  subject to relations of the form  $(s_i s_j)^{m_{ij}} = 1$  with  $m_{ij} = m_{ji} \geq 2$  for  $i \neq j$ .

The **finite** Coxeter groups have a **geometric representation** where the involutions are realised as **reflections** at **hyperplanes through the origin** in a Euclidean vector space  $\mathcal{E}$ . In particular, let  $(\cdot|\cdot)$  denote the inner product in  $\mathcal{E}$ , and  $v, \alpha \in \mathcal{E}$ .

The **generator**  $s_\alpha$  corresponds to the **reflection**

$$s_\alpha : v \rightarrow s_\alpha(v) = v - 2 \frac{(v|\alpha)}{(\alpha|\alpha)} \alpha$$

at a hyperplane perpendicular to the **root vector**  $\alpha$ .

The action of the **Coxeter group** is to permute these **root vectors**.

# Affine extensions

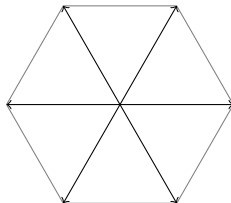
An **affine Coxeter group** is the extension of a Coxeter group by an **affine reflection in a hyperplane not containing the origin**  $s_{\alpha_0}^{aff}$  whose geometric action is given by

$$s_{\alpha_0}^{aff} v = \alpha_0 + v - \frac{2(\alpha_0 | v)}{(\alpha_0 | \alpha_0)} \alpha_0$$

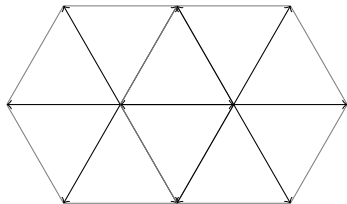
**Non-distance preserving:** includes the **translation generator**

$$Tv = v + \alpha_0 = s_{\alpha_0}^{aff} s_{\alpha_0} v$$

# Affine extensions – $A_2$

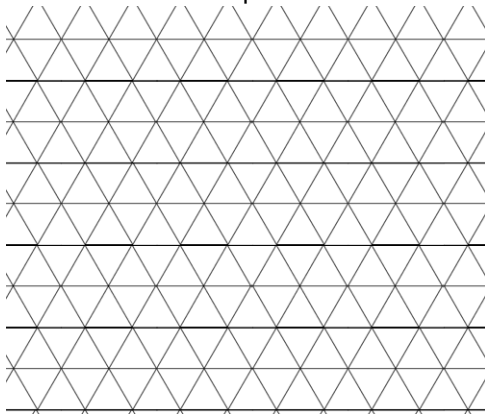


# Affine extensions – $A_2$



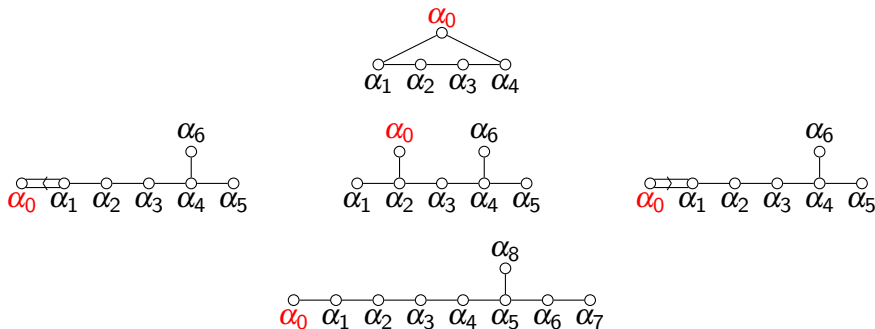
# Affine extensions – $A_2$

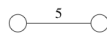
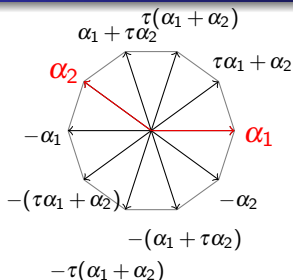
Affine extensions of crystallographic Coxeter groups lead to a **tessellation** of the plane and a **lattice**.



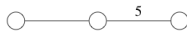


# Affine extensions of crystallographic groups $A_4$ , $D_6$ and $E_8$



Non-crystallographic Coxeter groups  $H_2 \subset H_3 \subset H_4$ 

$$A = \begin{pmatrix} 2 & -\tau \\ -\tau & 2 \end{pmatrix}$$



$$A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -\tau \\ 0 & -\tau & 2 \end{pmatrix}$$



$$A = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$H_2 \subset H_3 \subset H_4$ : 10, 120, 14,400 elements, the only Coxeter groups that generate **rotational symmetries of order 5**

linear combinations now in the **extended integer ring**

$$\mathbb{Z}[\tau] = \{a + \tau b \mid a, b \in \mathbb{Z}\} \quad \text{golden ratio}$$

$$\tau = \frac{1}{2}(1 + \sqrt{5}) = 2 \cos \frac{\pi}{5}$$

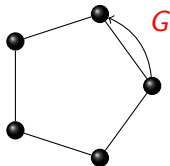
$$x^2 = x + 1$$

$$\tau' = \sigma = \frac{1}{2}(1 - \sqrt{5}) = 2 \cos \frac{2\pi}{5}$$

$$\tau + \sigma = 1, \tau\sigma = -1$$

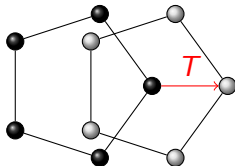
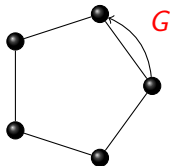
# Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



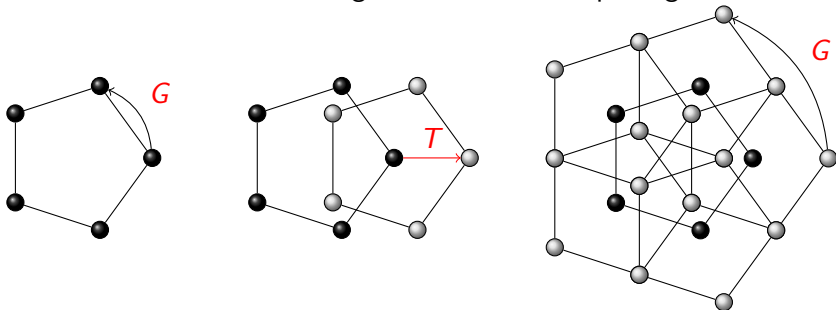
# Affine extensions of non-crystallographic root systems

Unit translation along a vertex of a unit pentagon



# Affine extensions of non-crystallographic root systems

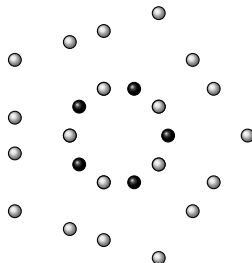
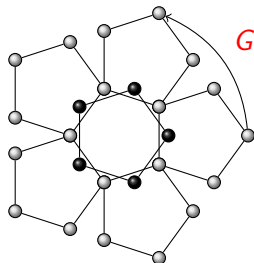
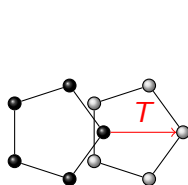
Unit translation along a vertex of a unit pentagon



A **random** translation would give 5 secondary pentagons, i.e. 25 points. Here we have **degeneracies** due to 'coinciding points'.

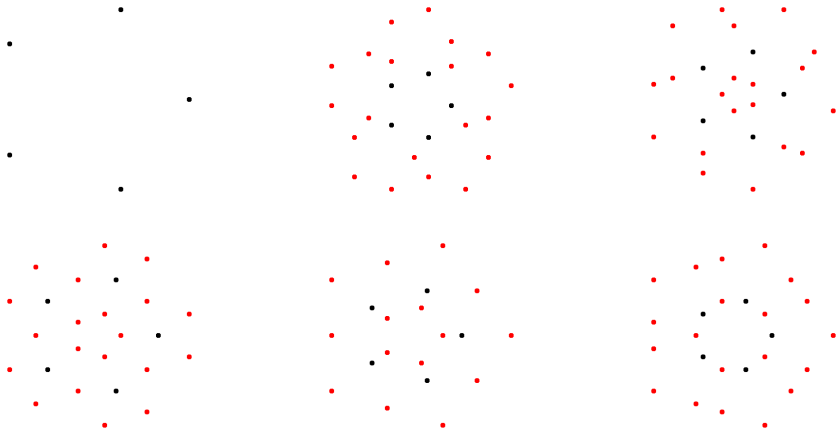
# Affine extensions of non-crystallographic root systems

Translation of length  $\tau = \frac{1}{2}(1 + \sqrt{5}) \approx 1.618$  (golden ratio)



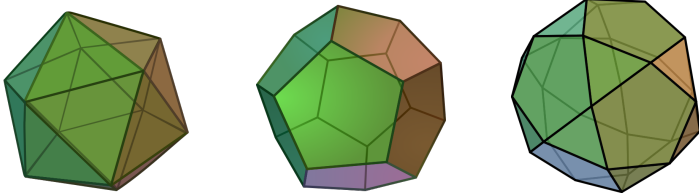
Looks like a **virus** or **carbon onion**

# More Blueprints



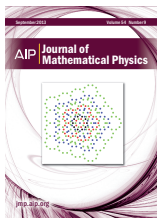
# Extend icosahedral group with distinguished translations

- Radial layers are **simultaneously constrained** by affine symmetry
- **Affine extensions** of the icosahedral group (giving translations) and their **classification**.





# Applications of affine extensions of non-crystallographic root systems



## Know your onions

Acta Cryst. A 70, 162-167 (2014)

Many viruses have icosahedral symmetry. So do certain carbon onions — Russian doll-like arrangements of nested fullerenes. Pierre-Philippe Dechant and colleagues argue that viruses and carbon onions share the same formation principle: affine symmetry.

Imagine a set of points lying on the vertices of a regular pentagon. Duplicate the set, and translate it; then repeatedly rotate the combined set over  $72^\circ$  about the midpoint of the original pentagon. This results in a new set of points obeying five-fold symmetry, yet with a 2D shell structure that is more complex than that of the pentagon. A similar ‘affinization’ of the (3D) icosahedral group results in a set of points that are nodes in the highly complex protein network structure of, for example, the Parvovirus.

Dechant *et al.* found that affine symmetry explains the structure of experimentally observed carbon onions — a non-trivial result given that all carbon atoms in each of the nested fullerene molecules must be three-connected; that is, bound to three neighbouring carbons. In particular, they identified the extended group that, starting from buckminsterfullerene (the ‘buckyball’), generates the onion  $C_{60} \otimes C_{240} \otimes C_{240}$ .

BV

well-known effect for photons, and it turns out to hold for other quantum particles too. James Fokema and colleagues have performed the Hong–Ou–Mandel quantum interference experiment using plasmons, which are quantized surface plasma waves. Pairs of photons are fed into a specially designed plasmonic waveguide that mixes the paths of the light-excited surface plasmons in the same way as a beam splitter. The outcome is converted back into photons and measured by two detectors. As in the purely photonic case, the characteristic dip in coincidence rate is there, showing that the photons remain indistinguishable when they are converted into plasmons and interfere. IG

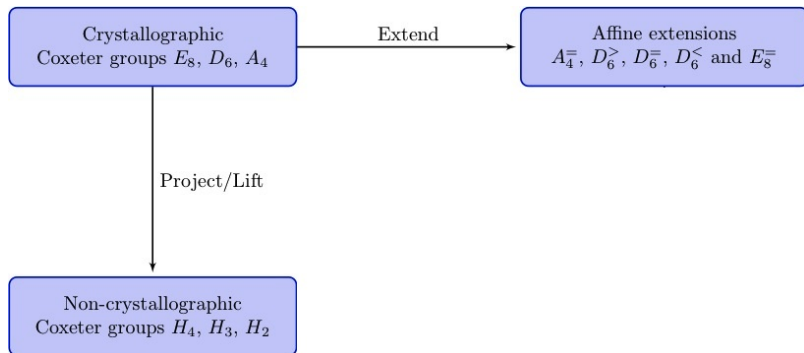
Written by May Chiao, Kater Gorenstein, Abigail Kopper, Bart Verbeek and Alison Wright

NATURE PHYSICS | VOL 10 | APRIL 2014 | www.nature.com/naturephysics

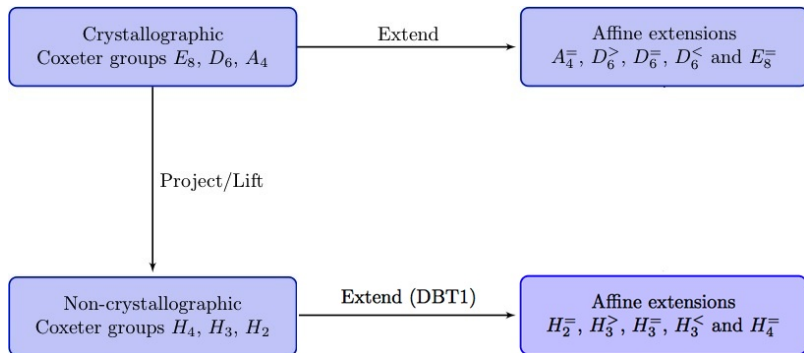
244

There are interesting applications to **quasicrystals**, **viruses** or **carbon onions** later, concentrate on the **mathematical** aspects for now

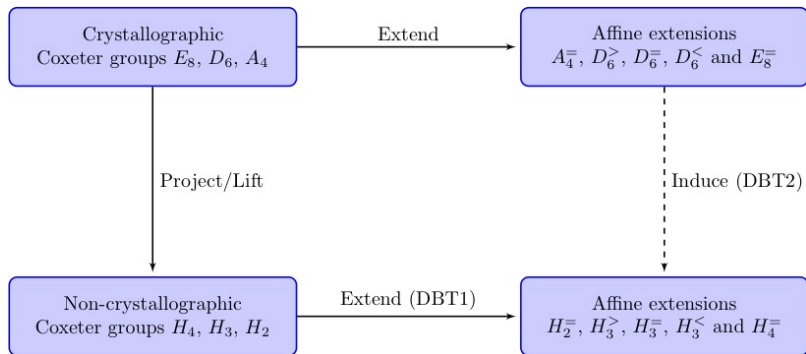
# Road Map



# Road Map



# Road Map



## 1 Affine extensions

- Direct extensions
- Induced extensions

## 2 Applications

- Virus Structure
- Fullerenes and Carbon onions

## 3 Conclusions

# Kac-Moody approach

Can recover these directly at the Cartan matrix level:

**Kac-Moody-type affine extension**  $A^{aff}$  of a Cartan matrix is an extension of the Cartan matrix  $A$  of a Coxeter group by further **rows**  $\underline{v}$  and **columns**  $\underline{w}$  such that:

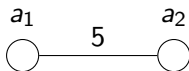
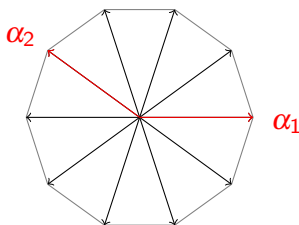
$$A^{aff} = \begin{pmatrix} 2 & \underline{v}^T \\ \underline{w} & A \end{pmatrix} \quad \boxed{A_{ii}^{aff} = 2} \quad \boxed{A_{ij}^{aff} \in \mathbb{Z}[\cdot]}$$

$$\boxed{A_{ij}^{aff} \leq 0} \quad \text{moreover,} \quad \boxed{A_{ij}^{aff} = 0 \Leftrightarrow A_{ji}^{aff} = 0}$$

$$\text{determinant constraint} \quad \boxed{\det A^{aff} = 0}$$

# Kac-Moody approach to $H_2$

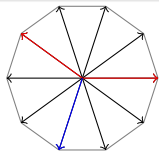
5



$$\alpha_1 = (1, 0), \quad \alpha_2 = \frac{1}{2}(-\tau, \sqrt{3-\tau})$$

$$A = \begin{pmatrix} 2 & \cdot & \cdot \\ \cdot & 2 & -\tau \\ \cdot & -\tau & 2 \end{pmatrix}$$

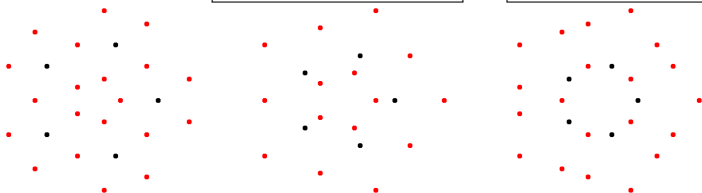
## Extension along the highest root



$$A = \begin{pmatrix} 2 & x & x \\ y & 2 & -\tau \\ y & -\tau & 2 \end{pmatrix}$$

$$xy = 2 - \tau = \sigma^2$$

symmetric  $x = y = \sigma = 1 - \tau$  recovers  $H_2^{aff}$  from Twarock et al  
new asymmetric e.g.  $(x, y) = (\tau - 2, -1)$  or  $(x, y) = (-1, \tau - 2)$



Write  $x = (a + \tau b)$  and  $y = (c + \tau d)$  with  $a, b, c, d \in \mathbb{Z}$ , i.e.  $H_2^{aff}$  is  $(a, b; c, d) = (1, -1; 1, -1)$ .



# Fibonacci scaling

The (non-trivial) **units** in  $\mathbb{Z}[\tau]$  are  $\tau^k$ ,  $k \in \mathbb{Z}$

Can **generate all solutions** to the determinant constraint  $xy = \sigma^2$   
by

**scaling**  $x \rightarrow \tau^{-k}x, y \rightarrow \tau^k y$ :  $xy$  invariant (giving the **angle**),  
but different **lengths**  $\sqrt{\frac{x}{y}} \rightarrow \sqrt{\frac{x}{y}}\tau^{-k}$

**Fibonacci scaling**

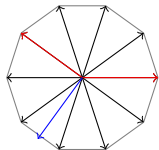
$(a, b; c, d) \rightarrow (b, a + b; d - c, c)$  for multiplication by  $(\tau, \tau^{-1})$  and

$(a, b; c, d) \rightarrow (b - a, a; d, c + d)$  for multiplication by  $(\tau^{-1}, \tau)$

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

**Swapping**  $x \leftrightarrow y$  generates another solution, but here symmetric

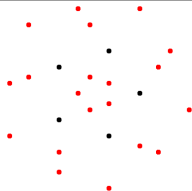
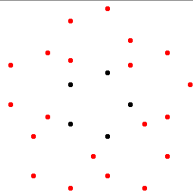
## Extension along a bisector



$$A = \begin{pmatrix} 2 & x & 0 \\ y & 2 & -\tau \\ 0 & -\tau & 2 \end{pmatrix}$$

$$xy = 3 - \tau$$

$$(x, y) = (\tau - 3, -1) \quad \text{or} \quad (x, y) = (-1, \tau - 3)$$



## 1 Affine extensions

- Direct extensions
- Induced extensions

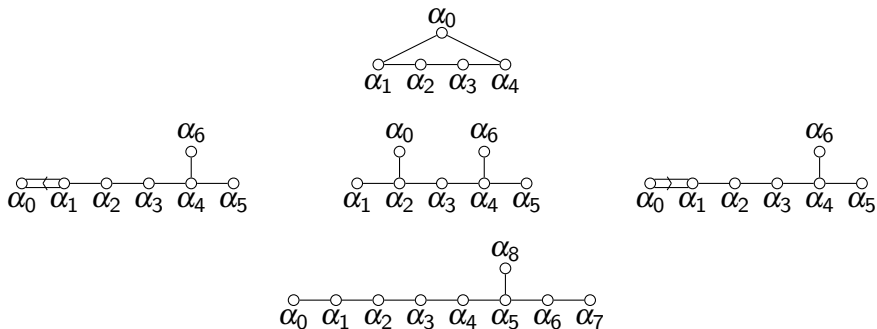
## 2 Applications

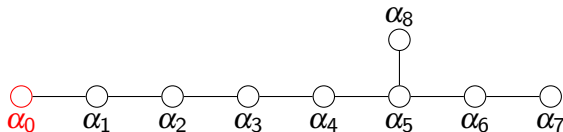
- Virus Structure
- Fullerenes and Carbon onions

## 3 Conclusions



# Recap: Affine extensions of crystallographic groups

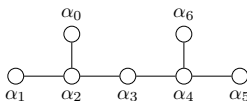


Affine extensions –  $E_8^-$ 

$$-\alpha_0 = 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8$$

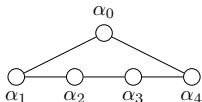
AKA  $E_8^+$  and along with  $E_8^{++}$  and  $E_8^{+++}$  thought to be the underlying symmetry of **String and M-theory**

Also interesting from a pure mathematics point of view:  **$E_8$  lattice**, **McKay correspondence** and **Monstrous Moonshine**.

Affine extensions – simply-laced  $D_6^=$ ,  $A_4^=$ 

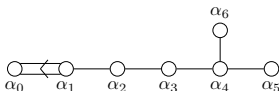
$$A(D_6^=) = \begin{pmatrix} 2 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$

$$-\alpha_0 = \alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6$$



$$A(A_4^=) = \begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

$$-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4$$

Affine extensions –  $D_6^<$  and  $D_6^>$ 

$$A(D_6^<) = \begin{pmatrix} 2 & -2 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$



$$A(D_6^>) = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ -2 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}$$

$$-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \frac{1}{2}\alpha_5 + \frac{1}{2}\alpha_6$$

$$-\alpha_0 = 2\alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6$$



Induced affine roots:  $H_4^-$  from  $E_8^-$ 

$$-\alpha_0 = 2\alpha_1 + 3\alpha_2 + 4\alpha_3 + 5\alpha_4 + 6\alpha_5 + 4\alpha_6 + 2\alpha_7 + 3\alpha_8$$

$$-a_0 = \pi_{\parallel}(-\alpha_0) = 2(1+\tau)a_1 + (3+4\tau)a_2 + 2(2+3\tau)a_3 + (3+5\tau)a_4$$

$$(a_1|a_2) = -\frac{1}{2}, (a_2|a_3) = -\frac{1}{2}, (a_3|a_4) = -\frac{\tau}{2},$$

$$A(H_4^-) := \begin{pmatrix} 2 & \tau-2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix}$$

induced affine root of lengths  $\tau$  and  $1/\tau$  along the highest root  $\alpha_H = (1, 0, 0, 0)$  of  $H_4$

Induced affine extensions:  $H_i^-$  from  $A_4^-$ ,  $D_6^-$  and  $E_8^-$ 

affine extensions of lengths  $\tau$  and  $1/\tau$  along the highest root  $\alpha_H$  of

$$A(H_4^-) := \begin{matrix} & H_i \\ \begin{pmatrix} 2 & \tau-2 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -\tau \\ 0 & 0 & 0 & -\tau & 2 \end{pmatrix} \end{matrix}$$

$$A(H_3^-) := \begin{pmatrix} 2 & 0 & \tau-2 & 0 \\ 0 & 2 & -1 & 0 \\ -1 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_2^-) := \begin{pmatrix} 2 & \tau-2 & \tau-2 \\ -1 & 2 & -\tau \\ -1 & -\tau & 2 \end{pmatrix}$$

Induced affine extensions: three  $H_3^+$  from  $D_6^+$ 

$$A(H_3^=) := \begin{pmatrix} 2 & 0 & \tau-2 & 0 \\ 0 & 2 & -1 & 0 \\ -1 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_3^<) := \begin{pmatrix} 2 & \frac{4}{5}(\tau-3) & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$A(H_3^>) := \begin{pmatrix} 2 & \frac{2}{5}(\tau-3) & 0 & 0 \\ -2 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

# Comparison with DBT1

- $H_i^{aff}$  was the **symmetric special case** of the **Fibonacci 'family' of solutions**
- $H_i^=$  **induced by projection** of the affine extensions  $E_8^=$ ,  $D_6^=$ ,  $A_4^=$  is the **'first asymmetric case'**
- Achieved by **scaling** the symmetric solution of  $H_i^{aff}$  by  $(\tau, \tau^{-1})$
- Projection from  $D_6^<$  and  $D_6^>$  give extensions along **5-fold axes** of icosahedral symmetry, from  $D_6^=$  along **2-fold axes**
- These are exactly what we were looking for for icosahedral applications!

## 1 Affine extensions

- Direct extensions
- Induced extensions

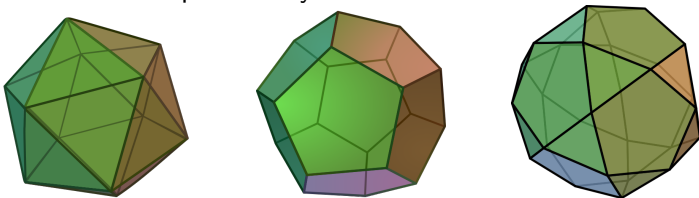
## 2 Applications

- Virus Structure
- Fullerenes and Carbon onions

## 3 Conclusions

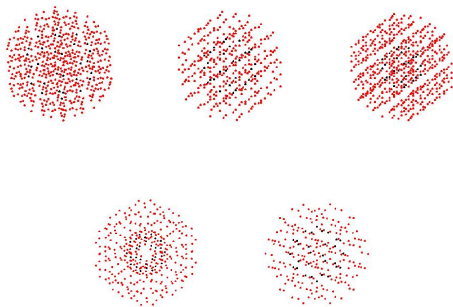
# Extend icosahedral group with distinguished translations

- Radial layers are **simultaneously constrained** by affine symmetry
- Works very well in practice: **finite library of blueprints**
- **Select** blueprint from the **outer shape** (capsid)
- Can **predict inner structure** (nucleic acid distribution) of the virus from the point array



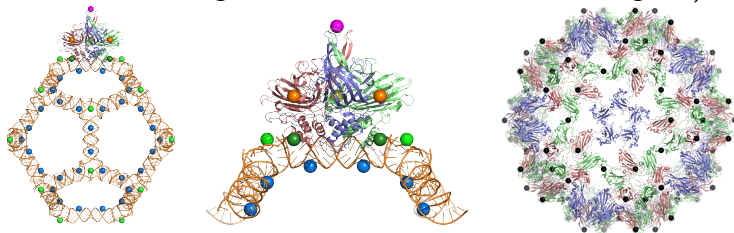
**Affine extensions** of the icosahedral group (giving translations) and their **classification**.

# What's the point?



# Use in Mathematical Virology

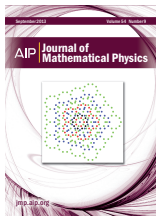
- Suffice to say **point arrays work very exceedingly well** in practice. Two papers on the mathematical (Coxeter) aspects.
- **Implemented computational problem in Clifford** – some **very interesting mathematics** comes out as well (see poster 'Platonic solids generate their 4-dimensional analogues').





# Use in Mathematical Virology

- Suffice to say **point arrays work very exceedingly well** in practice.
- Implemented computational problem in Clifford algebra** – some **very interesting mathematics** comes out as well (see poster ‘Platonic solids generate their 4-dimensional analogues’).



## Know your onions

Acta Cryst. A 70, 163-167 (2014)

Many viruses have icosahedral symmetry. So do certain ‘carbon onions’ — Russian doll-like arrangements of nested fullerenes. Pierre-Philippe Dechant and colleagues argue that viruses and carbon onions share the same formation principle: affine symmetry. Imagine a set of points lying on the vertices of a regular pentagon. Duplicate the set, and translate it, then repeatedly rotate the combined set over  $1/20$  about the midpoint of the original pentagon. This results in a new set of points obeying five-fold symmetry, yet with a 2D shell structure that is more complex than that of the pentagon. A similar affinitization of the 3D icosahedral group results in a set of points that are nodes in the highly complex protein network structure of, for example, the Pentaplex virus.

Dechant et al. found that affine symmetry explains the structure of experimentally observed carbon onions — a non-trivial result given that all carbon atoms in each of the nested fullerene molecules must be three-connected, that is, bound to three neighbouring carbons. In particular they identified the extended group that, starting from buckminsterfullerene (the ‘buckyball’), generates the onion  $C_{60}@C_{60}@C_{60}$ .

well-known effect for photons, and it turns out to hold for other quantum particles too. James Pakevas and colleagues have performed the Hong–Ou–Mandel quantum interference experiment using plasmons, which are quantized surface plasma waves. Pairs of photons are fed into a specially designed plasmonic waveguide that mixes the paths of the light-excited surface plasmons in the same way as a beam splitter. The outcome is converted back into photons and measured by two detectors. As in the purely photonic case, the characteristic dip in coincidence rate is there, showing that the photons remain indistinguishable when they are converted into plasmons and interfere.

Written by Amy Chow, Kiko Georgescu, Abigail Knappe, Bert Verbruggen and Ahsan ul-Haque

BY

NATURE PHYSICS | VOL 10 | APRIL 2014 | www.nature.com/naturephysics

244

## 1 Affine extensions

- Direct extensions
- Induced extensions

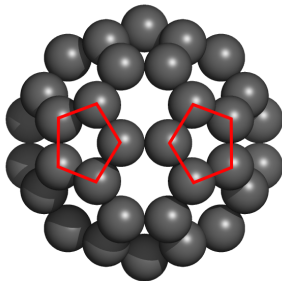
## 2 Applications

- Virus Structure
- Fullerenes and Carbon onions

## 3 Conclusions

# Constraints of carbon chemistry

- Relevant carbon bonding here is **trivalent**
- **Bond lengths and angles** need to be pretty **uniform**
- For example, the well-known **football-shaped** Buckyball  $C_{60}$



# Strategy

- Extend icosahedral shapes with a **translation** and take orbit under the compact group
- Select **outer shells** that are **three-coordinated** and uniform enough
- For the usual **icosahedron, dodecahedron, icosidodecahedron** find few not very interesting possibilities
- For  **$C_{60}$  and  $C_{80}$**  start, get a **unique** extension that exactly give the known **carbon onions**  $C_{60} - C_{240} - C_{540}$  and  $C_{80} - C_{180} - C_{320}$

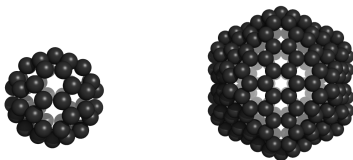
# Fullerene cages derived from $C_{60}$

- Extend idea of affine symmetry to other objects in nature: icosahedral **fullerenes**
- Recover different shells with icosahedral symmetry from affine approach starting with  $C_{60}$ : **carbon onion** ( $C_{60} - C_{240} - C_{540}$ )



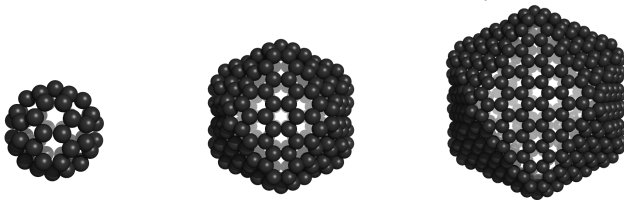
# Fullerene cages derived from $C_{60}$

- Extend idea of affine symmetry to other objects in nature: icosahedral **fullerenes**
- Recover different shells with icosahedral symmetry from affine approach starting with  $C_{60}$ : **carbon onion** ( $C_{60} - C_{240} - C_{540}$ )



# Fullerene cages derived from $C_{60}$

- Extend idea of affine symmetry to other objects in nature: icosahedral **fullerenes**
- Recover different shells with icosahedral symmetry from affine approach starting with  $C_{60}$ : **carbon onion** ( $C_{60} - C_{240} - C_{540}$ )



# Fullerene cages derived from $C_{80}$

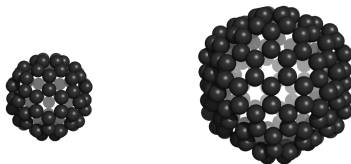
- Extend idea of affine symmetry to other objects in nature: icosahedral **fullerenes**
- Recover different shells with icosahedral symmetry from affine approach starting with  $C_{80}$ : **carbon onion** ( $C_{80} - C_{180} - C_{320}$ )





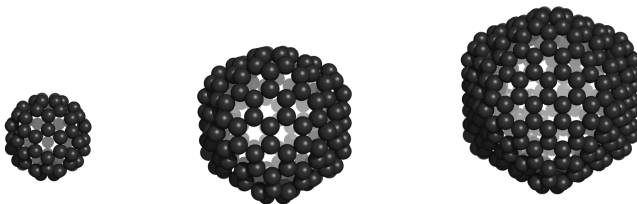
# Fullerene cages derived from $C_{80}$

- Extend idea of affine symmetry to other objects in nature: icosahedral **fullerenes**
- Recover different shells with icosahedral symmetry from affine approach starting with  $C_{80}$ : **carbon onion** ( $C_{80} - C_{180} - C_{320}$ )



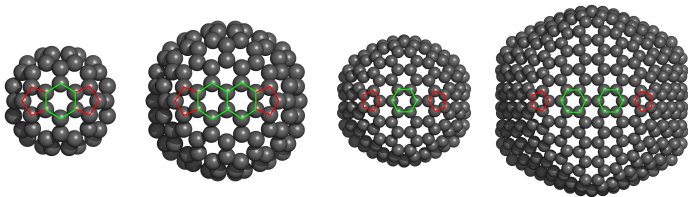
# Fullerene cages derived from $C_{80}$

- Extend idea of affine symmetry to other objects in nature: icosahedral **fullerenes**
- Recover different shells with icosahedral symmetry from affine approach starting with  $C_{80}$ : **carbon onion** ( $C_{80} - C_{180} - C_{320}$ )



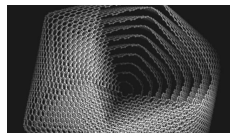
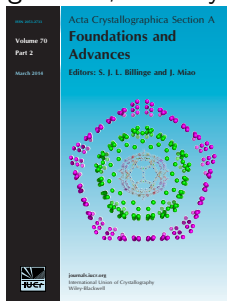
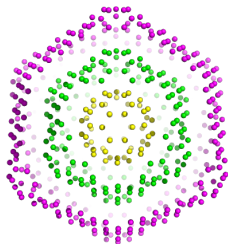
# Growth of shells by a hexamer at a time

- Hence, for  $C_{60}$  and  $C_{80}$  start, get a **unique** extension that exactly give the known **carbon onions**  $C_{60} - C_{240} - C_{540}$  and  $C_{80} - C_{180} - C_{320}$  by inserting an **additional hexamer** at each step



# Viruses and fullerenes – symmetry as a common thread?

- Get nested arrangements like Russian dolls: **carbon onions** (e.g. June: Nature 510, 250253)
- Potential to extend to **other known carbon onions** with different start configuration, chirality etc



# References (collaborations)

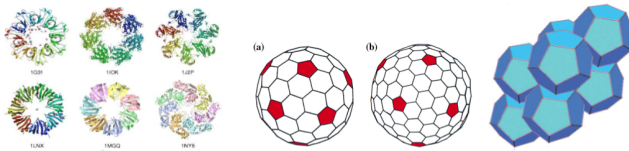
- Novel Kac-Moody-type affine extensions of non-crystallographic Coxeter groups with Twarock/Bøhm J. Phys. A: Math. Theor. 45 285202 (2012)
- Affine extensions of non-crystallographic Coxeter groups induced by projection with Twarock/Bøhm Journal of Mathematical Physics 54 093508 (2013), [Cover article September](#)
- Viruses and Fullerenes – Symmetry as a Common Thread? with Twarock/Wardman/Keef Acta Crystallographica A 70 (2). pp. 162-167 (2014), [Cover article March](#), [Nature Physics Research Highlight](#)

# References (single-author)

- Clifford algebra unveils a surprising geometric significance of quaternionic root systems of Coxeter groups  
Advances in Applied Clifford Algebras 23 (2). pp. 301-321 (2013)
- A Clifford algebraic framework for Coxeter group theoretic computations (Conference Prize at AGACSE 2012)  
Advances in Applied Clifford Algebras 24 (1). pp. 89-108 (2014)
- Rank-3 root systems induce root systems of rank 4 via a new Clifford spinor construction arXiv:1207.7339 (2012)
- Platonic Solids generate their 4-dimensional analogues  
Acta Cryst. A69 (2013)

# Conclusions

- Novel mathematical structures
- Interesting in their own right
- Numerous applications to real systems: Viruses, Proteins, Fullerenes, Quasicrystals, Tilings, Packings etc.
- Potential applications to engineering and medicine: nanotechnology and drug delivery



Thank you!

(For a construction that induces from every rank 3 root system a rank 4 root system via Clifford spinors, see my poster)



Extension along the highest root – two-fold axis  $T_2$ 

$$\alpha_1 = (0, 1, 0), \alpha_2 = -\frac{1}{2}(-\sigma, 1, \tau), \alpha_3 = (0, 0, 1)$$

$$T_2 = (1, 0, 0)$$

$$A = \begin{pmatrix} 2 & 0 & x & 0 \\ 0 & 2 & -1 & 0 \\ y & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$xy = \sigma^2 = 2 - \tau$$

Same solution as in the previous case of  $H_2$ .

Extension along a three-fold axis  $T_3$ 

$$\alpha_1 = (0, 1, 0), \quad \alpha_2 = -\frac{1}{2}(-\sigma, 1, \tau), \quad \alpha_3 = (0, 0, 1)$$

$$T_3 = (\tau, 0, \sigma)$$

$$A = \begin{pmatrix} 2 & 0 & 0 & x \\ 0 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ y & 0 & -\tau & 2 \end{pmatrix}$$

$$xy = \frac{4}{3}\sigma^2$$

No longer  $\mathbb{Z}[\tau]$ -valued, and hence **solutions do not exist in  $\mathbb{Z}[\tau]$** .  
What now? Allow  $\mathbb{Q}[\tau]$ ? Write  $x = \gamma(a + \tau b)$  and  $y = \delta(c + \tau d)$

with  $a, b, c, d \in \mathbb{Z}$  and  $\gamma, \delta \in \mathbb{Q}$ . Need  $\gamma\delta = \frac{4}{3}$ , then can recycle  
integer solution

Extension along a five-fold axis  $T_5$ 

$$\alpha_1 = (0, 1, 0), \alpha_2 = -\frac{1}{2}(-\sigma, 1, \tau), \alpha_3 = (0, 0, 1)$$

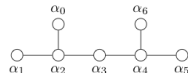
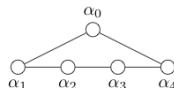
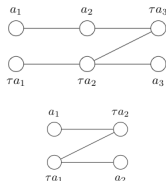
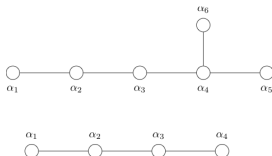
$$T_5 = (\tau, -1, 0)$$

$$A = \begin{pmatrix} 2 & x & 0 & 0 \\ y & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$$xy = \frac{4}{5}(3 - \tau)$$

Same solution (two series) as before in the case of  $H_2$ , but this time with the additional degree of freedom.

# Invariance under Dynkin diagram automorphisms



$$-\alpha_0 = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4$$

$$-\alpha_0 = \alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6$$

$$-\alpha_0 = 2\alpha_1 + 2\alpha_2 + 2\alpha_3 + 2\alpha_4 + \alpha_5 + \alpha_6$$